

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1743MXC

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	DEC 21	IPC search and display fields enhanced in CA/CAPLUS with the IPC reform
NEWS	4	DEC 23	New IPC8 SEARCH, DISPLAY, and SELECT fields in USPATFULL/USPAT2
NEWS	5	JAN 13	IPC 8 searching in IFIPAT, IFIUDB, and IFICDB
NEWS	6	JAN 13	New IPC 8 SEARCH, DISPLAY, and SELECT enhancements added to INPADOC
NEWS	7	JAN 17	Pre-1988 INPI data added to MARPAT
NEWS	8	JAN 17	IPC 8 in the WPI family of databases including WPIFV
NEWS	9	JAN 30	Saved answer limit increased
NEWS	10	JAN 31	Monthly current-awareness alert (SDI) frequency added to TULSA
NEWS	11	FEB 21	STN AnaVist, Version 1.1, lets you share your STN AnaVist visualization results
NEWS	12	FEB 22	Status of current WO (PCT) information on STN
NEWS	13	FEB 22	The IPC thesaurus added to additional patent databases on STN
NEWS	14	FEB 22	Updates in EPFULL; IPC 8 enhancements added
NEWS	15	FEB 27	New STN AnaVist pricing effective March 1, 2006
NEWS	16	FEB 28	MEDLINE/LMEDLINE reload improves functionality
NEWS	17	FEB 28	TOXCENTER reloaded with enhancements
NEWS	18	FEB 28	REGISTRY/ZREGISTRY enhanced with more experimental spectral property data
NEWS	19	MAR 01	INSPEC reloaded and enhanced
NEWS	20	MAR 03	Updates in PATDPA; addition of IPC 8 data without attributes
NEWS	21	MAR 08	X.25 communication option no longer available after June 2006
NEWS EXPRESS			FEBRUARY 15 CURRENT VERSION FOR WINDOWS IS V8.01a, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 19 DECEMBER 2005. V8.0 AND V8.01 USERS CAN OBTAIN THE UPGRADE TO V8.01a AT http://download.cas.org/express/v8.0-Discover/
NEWS HOURS			STN Operating Hours Plus Help Desk Availability
NEWS LOGIN			Welcome Banner and News Items

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 19:36:10 ON 19 MAR 2006

=> file registry
COST IN U.S. DOLLARS
FULL ESTIMATED COST

SINCE FILE ENTRY	TOTAL SESSION
0.21	0.21

FILE 'REGISTRY' ENTERED AT 19:36:16 ON 19 MAR 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2006 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 17 MAR 2006 HIGHEST RN 877201-63-3
DICTIONARY FILE UPDATES: 17 MAR 2006 HIGHEST RN 877201-63-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

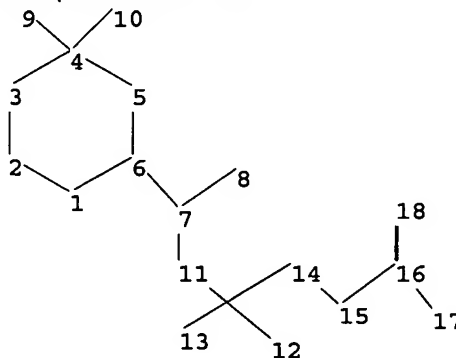
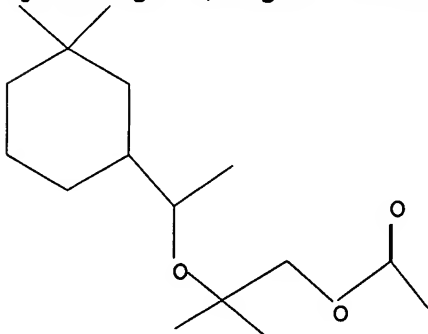
*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*

Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>
Uploading C:\Program Files\Stnexp\Queries\10792375.str



chain nodes :

7 8 9 10 11 12 13 14 15 16 17 18

ring nodes :

1 2 3 4 5 6

chain bonds :

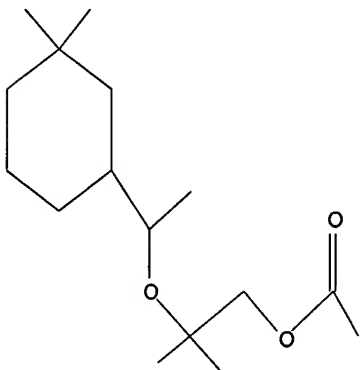
4-9 4-10 6-7 7-8 7-11 11-12 13-14 14-15 15-16 16-17 16-18

ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-11 11-12 14-15 15-16 16-18
exact bonds :
4-9 4-10 6-7 7-8 13-14 16-17

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss full
FULL SEARCH INITIATED 19:36:37 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 22543 TO ITERATE

100.0% PROCESSED 22543 ITERATIONS 7 ANSWERS
SEARCH TIME: 00.00.01

L2 7 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS
FULL ESTIMATED COST

SINCE FILE	TOTAL
ENTRY	SESSION
	

FILE 'CAPLUS' ENTERED AT 19:36:41 ON 19 MAR 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching

databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 19 Mar 2006 VOL 144 ISS 13
FILE LAST UPDATED: 17 Mar 2006 (20060317/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

=> s 12

L3 3 L2

=> d l3 1-3 hitstr, ibib, iabs

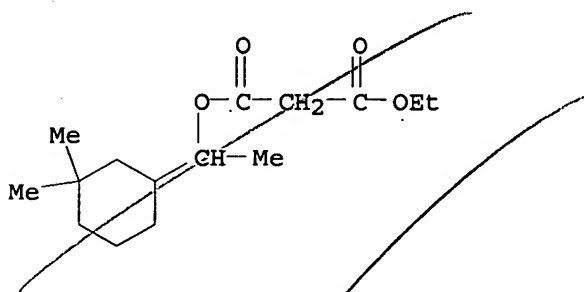
L3 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN

IT 478695-70-4P 670224-85-8P

RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(fruity musk compns. comprising ester compds.)

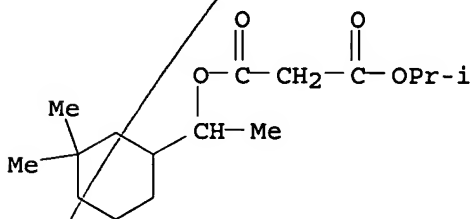
RN 478695-70-4 CAPLUS

CN Propanedioic acid, 1-(3,3-dimethylcyclohexyl)ethyl ethyl ester (9CI) (CA INDEX NAME)



RN 670224-85-8 CAPLUS

CN Propanedioic acid, 1-(3,3-dimethylcyclohexyl)ethyl 1-methylethyl ester (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 2004:214748 CAPLUS

DOCUMENT NUMBER: 140:258663

TITLE: Fruity musk compositions comprising ester compounds
INVENTOR(S): Bledsoe, James O.; Britten-Kelly, Michael; Sprecker, Mark A.; Belko, Robert P.; Pawlak, Manfred; Monteleone, Michael G.

PATENT ASSIGNEE(S): International Flavors & Fragrances Inc., USA

SOURCE: Eur. Pat. Appl., 10 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1398366	A1	20040317	EP 2003-255719	20030912
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
US 2004053811	A1	20040318	US 2002-243143	20020914
US 6774260	B2	20040810		
US 2004209796	A1	20041021	US 2004-846456	20040514
US 2004214745	A1	20041028	US 2004-845935	20040514
US 6919477	B2	20050719		

PRIORITY APPLN. INFO.:

US 2002-243143 A 20020914

OTHER SOURCE(S):

MARPAT 140:258663

ABSTRACT:

Novel ester compds. and the use of these esters as a fragrance chems., suitable for use in creating fragrance, and scents in items such as perfumes, colognes and personal care products are disclosed. Ethyl-1-(3,3-dimethylcyclohexyl) Et malonate (I) was prepared by the reaction of di-Et malonate alpha-3,3-trimethylcyclohexanemethanol. Fragrance formulations containing I are disclosed.

REFERENCE COUNT:

4

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN

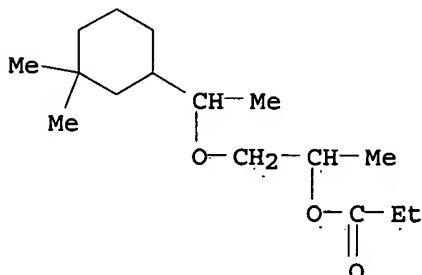
IT 141773-62-8P 141773-64-0P 141773-67-3P

141773-72-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as perfume fragrance)

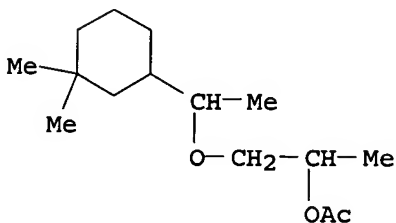
RN 141773-62-8 CAPLUS

CN 2-Propanol, 1-[1-(3,3-dimethylcyclohexyl)ethoxy]-, propanoate (9CI) (CA INDEX NAME)



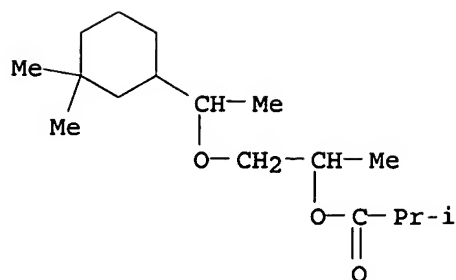
RN 141773-64-0 CAPLUS

CN 2-Propanol, 1-[1-(3,3-dimethylcyclohexyl)ethoxy]-, acetate (9CI) (CA INDEX NAME)

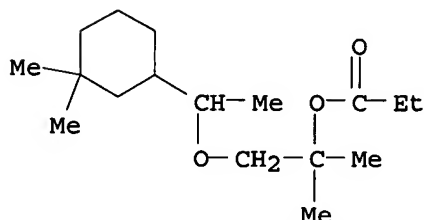


RN 141773-67-3 CAPLUS

CN Propanoic acid, 2-methyl-, 2-[1-(3,3-dimethylcyclohexyl)ethoxy]-1-methylethyl ester (9CI) (CA INDEX NAME)



RN 141773-72-0 CAPLUS
 CN 2-Propanol, 1-[1-(3,3-dimethylcyclohexyl)ethoxy]-2-methyl-, propanoate
 (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1992:407513 CAPLUS
 DOCUMENT NUMBER: 117:7513
 TITLE: Preparation of 4-cycloalkyl-3-oxapentyl alkanooates as
 perfume fragrances
 INVENTOR(S): Giersch, Wolfgang Klaus; Schulte-Elte, Karl Heinrich
 PATENT ASSIGNEE(S): Firmenich S. A., Switz.
 SOURCE: Eur. Pat. Appl., 15 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: French
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 472966	A1	19920304	EP 1991-113240	19910807
EP 472966	B1	19940928		
R: CH, DE, FR, GB, LI, NL				
US 5166412	A	19921124	US 1991-741027	19910806
JP 06072952	A2	19940315	JP 1991-214881	19910827
JP 2974834	B2	19991110		

PRIORITY APPLN. INFO.: CH 1990-2799 A 19900828
 OTHER SOURCE(S): MARPAT 117:7513

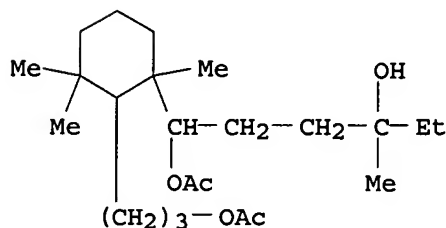
ABSTRACT:

RCHMeOCR1R2CR3R4O2CR5 (R = 3,3-dimethylcyclopentyl, -cyclohexyl; when R1 = R2 = H, R3 and/or R4 = Me; when R3 = R4 = H, R1 and/or R2 = Me; R5 = alkyl) were prepared. Thus, 1-(3,3-dimethyl-1-cyclohexyl)-1-ethanone was ketalized by HOCH2CHMeOH and the dioxolane product reduced with Dibal to give RCHMeOCHMeCH2OR4 (I; R = 3,3-dimethylcyclohexyl) (II; R4 = H) and RCHMeOCH2CHMeOR4 (III; R same as I) (IV; R4 = H) as a mixture which was treated with EtCOCl to give II and IV (R4 = EtCO in each) as mixts. of diastereomers. Perfume formulations comprising title compds. are given.

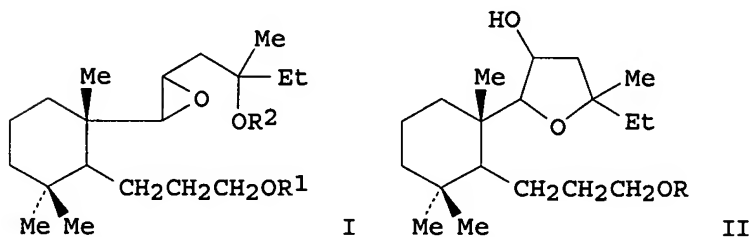
L3 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN
 IT 134427-57-9P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (preparation and carbon-13 NMR of)

RN 134427-57-9 CAPLUS
 CN 1,4-Hexanediol, 1-[2-[3-(acetyloxy)propyl]-1,3,3-trimethylcyclohexyl]-4-methyl-, 1-acetate, [1S-[1 α (1R*,4R*),2 β]]- (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1991:429666 CAPLUS
 DOCUMENT NUMBER: 115:29666
 TITLE: Intramolecular participation reactions in labda-8(17),14-dien-13-ol (manool) derivatives
 AUTHOR(S): Grant, Peter K.; Hanton, Lyall R.; Tsai, Siew Fah; Yap, Tho Man
 CORPORATE SOURCE: Dep. Chem., Univ. Otago, Dunedin, N. Z.
 SOURCE: Australian Journal of Chemistry (1991), 44(3), 433-46
 CODEN: AJCHAS; ISSN: 0004-9425
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 115:29666
 GRAPHIC IMAGE:



ABSTRACT:

Lewis acid treatment of a series of hydroxy epoxides, e.g., I (R1 = R2 = H, R1 = Ac, R2 = H) promoted intramol. nucleophilic epoxide opening to give hydroxy cyclic ethers II. The regioselectivity of epoxide opening is controlled by a preference for SN2 attack at the more accessible epoxide carbon, provided this does not involve the formation of a strained ether ring. An intramol. acetate transfer occurs in order to achieve the regioselective opening.

=> file registry
 COST IN U.S. DOLLARS

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

CA SUBSCRIBER PRICE

SINCE FILE ENTRY	TOTAL SESSION
SINCE FILE ENTRY	TOTAL SESSION
-2.25	-2.25

FILE 'REGISTRY' ENTERED AT 19:40:53 ON 19 MAR 2006
 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2006 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 17 MAR 2006 HIGHEST RN 877201-63-3
DICTIONARY FILE UPDATES: 17 MAR 2006 HIGHEST RN 877201-63-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

```
*****
*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*
*****
```

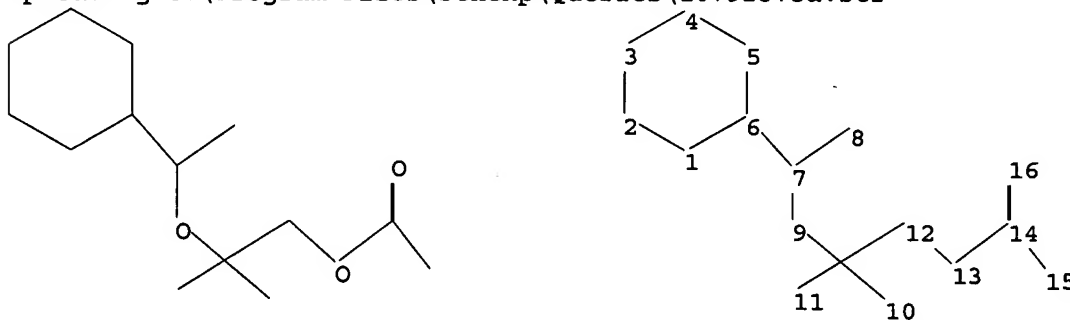
Structure search iteration limits have been increased. See HELP SLIMITS
for details.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10792375a.str



```
chain nodes :
7 8 9 10 11 12 13 14 15 16
ring nodes :
1 2 3 4 5 6
chain bonds :
6-7 7-8 7-9 9-10 11-12 12-13 13-14 14-15 14-16
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-9 9-10 12-13 13-14 14-16
exact bonds :
6-7 7-8 11-12 14-15
```

Match level :

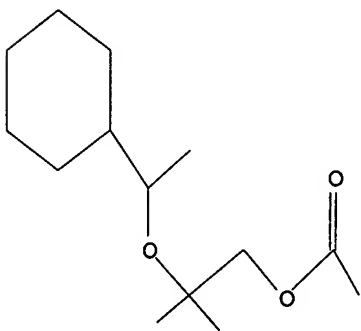
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS

L4 STRUCTURE UPLOADED

=> d 14

L4 HAS NO ANSWERS

L4 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 14 sss full

FULL SEARCH INITIATED 19:41:37 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 354062 TO ITERATE

100.0% PROCESSED 354062 ITERATIONS

6131 ANSWERS

SEARCH TIME: 00.00.03

L5 6131 SEA SSS FUL L4

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

0.00

-2.25

FILE 'CAPLUS' ENTERED AT 19:41:46 ON 19 MAR 2006

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 19 Mar 2006 VOL 144 ISS 13

FILE LAST UPDATED: 17 Mar 2006 (20060317/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

<http://www.cas.org/infopolicy.html>

=> s 15

L6 2590 L5

=> s 16 and (perfum? or fragran? or odor? or smell or olfactor?)

33422 PERFUM?

14984 FRAGRAN?

85650 ODOR?

5701 SMELL

646 SMELLS

6200 SMELL

(SMELL OR SMELLS)

18036 OLFACTOR?

L7 20 L6 AND (PERFUM? OR FRAGRAN? OR ODOR? OR SMELL OR OLFACTOR?)

=> d 17 1-20 hitstr, ibib, iabs

L7 ANSWER 1 OF 20 CAPLUS COPYRIGHT 2006 ACS on STN

IT 101007-06-1

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL

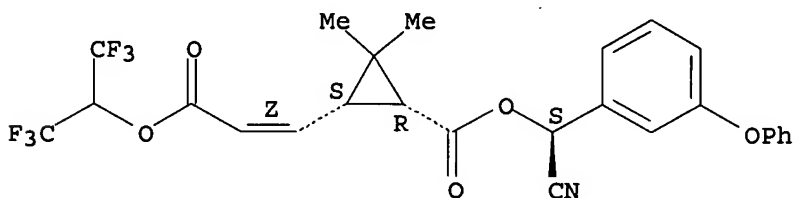
(Biological study); USES (Uses)

(methods and compns. for increasing efficacy of biol. active
ingredients such as antitumor agents)

RN 101007-06-1 CAPLUS

CN Cyclopropanecarboxylic acid, 2,2-dimethyl-3-[(1Z)-3-oxo-3-[2,2,2-trifluoro-
1-(trifluoromethyl)ethoxy]-1-propenyl]-, (S)-cyano(3-phenoxyphenyl)methyl
ester, (1R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



ACCESSION NUMBER: 2005:141200 CAPLUS

DOCUMENT NUMBER: 142:254568

TITLE: Methods and compositions for increasing the efficacy
of biologically-active ingredients such as antitumor
agents

INVENTOR(S): Windsor, J. Brian; Roux, Stan J.; Lloyd, Alan M.;
Thomas, Collin E.

PATENT ASSIGNEE(S): Board of Regents, the University of Texas System, USA

SOURCE: PCT Int. Appl., 243 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005014777	A2	20050217	WO 2003-US32667	20031016
WO 2005014777	A3	20050915		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

CA 2502148 AA 20050217 CA 2003-2502148 20031016

EP 1576150 A2 20050921 EP 2003-816736 20031016

EP 1576150 A3 20051102

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK

PRIORITY APPLN. INFO.:

US 2002-418803P P 20021016

WO 2003-US32667 W 20031016

ABSTRACT:

The invention provides methods and compns. for modulating the sensitivity of cells to cytotoxic compds. and other active agents. In accordance with the invention, compns. are provided comprising combinations of ectophosphatase inhibitors and active agents. Active agents include antibiotics, fungicides, herbicides, insecticides, chemotherapeutic agents, and plant growth regulators. By increasing the efficacy of active agents, the invention allows use of compns. with lowered concns. of active ingredients.

L7 ANSWER 2 OF 20 CAPLUS COPYRIGHT 2006 ACS on STN

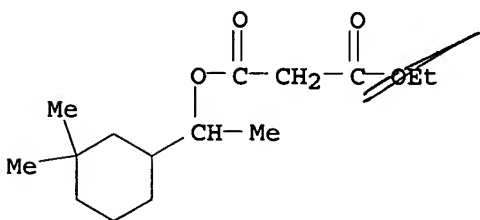
IT 478695-70-4P 670224-85-8P

RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(fruity musk compns. comprising ester compds.)

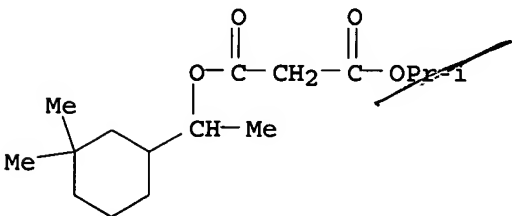
RN 478695-70-4 CAPLUS

CN Propanedioic acid, 1-(3,3-dimethylcyclohexyl)ethyl ethyl ester (9CI) (CA INDEX NAME)



RN 670224-85-8 CAPLUS

CN Propanedioic acid, 1-(3,3-dimethylcyclohexyl)ethyl 1-methylethyl ester (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 2004:214748 CAPLUS

DOCUMENT NUMBER: 140:258663

TITLE: Fruity musk compositions comprising ester compounds

INVENTOR(S): Bledsoe, James O.; Britten-Kelly, Michael; Sprecker, Mark A.; Belko, Robert P.; Pawlak, Manfred; Monteleone, Michael G.
 PATENT ASSIGNEE(S): International Flavors & Fragrances Inc., USA
 SOURCE: Eur. Pat. Appl., 10 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

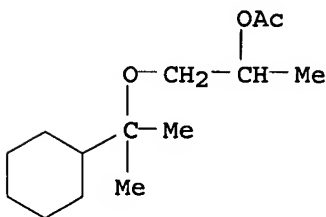
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1398366	A1	20040317	EP 2003-255719	20030912
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
US 2004053811	A1	20040318	US 2002-243143	20020914
US 6774260	B2	20040810		
US 2004209796	A1	20041021	US 2004-846456	20040514
US 2004214745	A1	20041028	US 2004-845935	20040514
US 6919477	B2	20050719		
PRIORITY APPLN. INFO.:			US 2002-243143	A 20020914
OTHER SOURCE(S):	MARPAT 140:258663			

ABSTRACT:

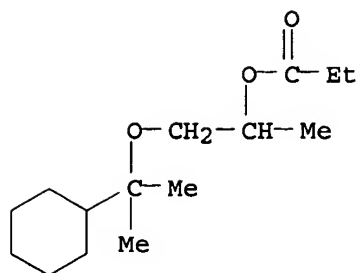
Novel ester compds. and the use of these esters as a **fragrance** chems., suitable for use in creating **fragrance**, and scents in items such as **perfumes**, colognes and personal care products are disclosed. Ethyl-1-(3,3-dimethylcyclohexyl) Et malonate (I) was prepared by the reaction of di-Et malonate alpha-3,3-trimethylcyclohexanemethanol. **Fragrance** formulations containing I are disclosed.

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 3 OF 20 CAPLUS COPYRIGHT 2006 ACS on STN
 IT 610770-07-5P 610770-08-6P
 RL: COS (Cosmetic use); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of novel alicyclic esters having a musky **smell**)
 RN 610770-07-5 CAPLUS
 CN 2-Propanol, 1-(1-cyclohexyl-1-methylethoxy)-, acetate (9CI) (CA INDEX NAME)

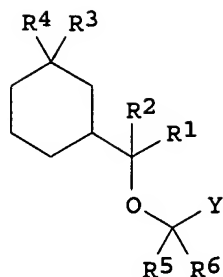


RN 610770-08-6 CAPLUS
 CN 2-Propanol, 1-(1-cyclohexyl-1-methylethoxy)-, propanoate (9CI) (CA INDEX NAME)

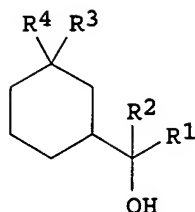


ACCESSION NUMBER: 2003:796643 CAPLUS
 DOCUMENT NUMBER: 139:307907
 TITLE: Methods for the production of novel alicyclic esters having a musky smell
 INVENTOR(S): Eh, Marcus
 PATENT ASSIGNEE(S): Symrise GmbH & Co. KG, Germany
 SOURCE: PCT Int. Appl., 45 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

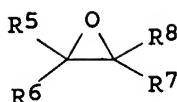
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003082799	A2	20031009	WO 2003-EP3294	20030329
WO 2003082799	A3	20031231		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10214675	A1	20031016	DE 2002-10214675	20020403
AU 2003239793	A1	20031013	AU 2003-239793	20030329
BR 2003004218	A	20040727	BR 2003-4218	20030329
EP 1492759	A2	20050105	EP 2003-732270	20030329
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
US 2005182273	A1	20050818	US 2003-510024	20030329
PRIORITY APPLN. INFO.: DE 2002-10214675 A 20020403 WO 2003-EP3294 W 20030329				
OTHER SOURCE(S): CASREACT 139:307907; MARPAT 139:307907				
GRAPHIC IMAGE:				



I



II



III

ABSTRACT:

The invention relates to novel alicyclic esters I [R1 = Me; R2, R4 = H; R3 = H, Me; R5, R6 = H, Me; Y = CR7R8OC(:O)R9; R7, R8 = H, Me; R9 = C1-5-alkyl, C2-5-alkylene; or R1, R2 = Me, Et; R3, R4 = H, Me; R5R6 = O; Y = CR7R8OC(:O)R9; or R1, R2 = Me, Et; R4, R5, R6, R7 = H, Me; Y = CR7R8OC(:O)R9], methods for their production, for their use as **odorous** substances for ***perfumed*** products and for **odorous** substance mixts. containing the inventive compds. The procedure for the preparation of I is characterized by reaction of cyclohexylalkanols II with carboxylic acids [R9CO2CR7R8CO2H, R9CO2H or XCR7R8CO2H (X = OH, halogen)] anhydrides [(R9CO2)2O or (XCR7R8CO2)2O], or epoxides, III. Thus, I [R1 = Me, R2 - R4 = H, R6 = CHMe2, Y = O2CET] was prepared from 1-cyclohexylethanol via reaction with isobutylene oxide in cyclohexane containing BF3·OEt2, followed by reaction with (EtCO2)2O containing Et3N in the presence of catalytic DMAP. The **odor** of I [R1 = Me, R2 - R4 = H, R6 = CHMe2, Y = O2CET] was characterized (perceptible rose bloom note).

L7 ANSWER 4 OF 20 CAPLUS COPYRIGHT 2006 ACS on STN

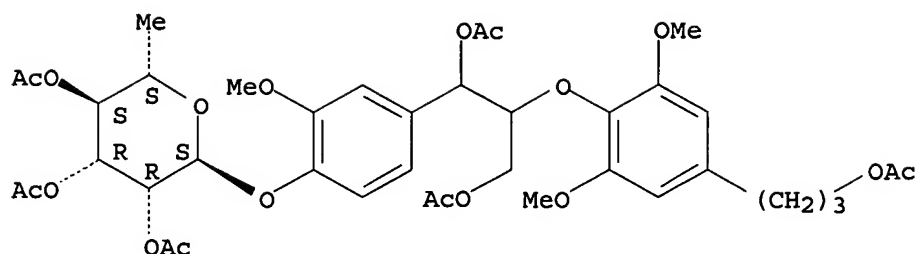
IT 524938-05-4P, Nymphaeoside A peracetate

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and properties of)

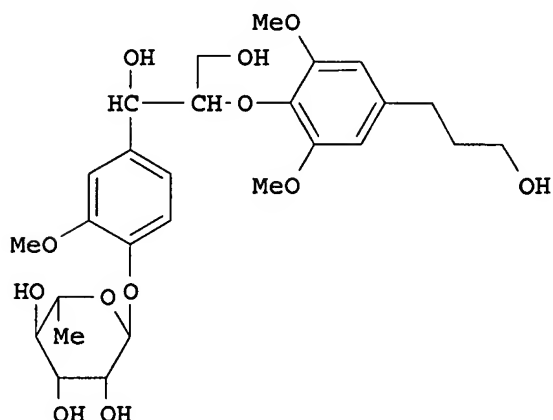
RN 524938-05-4 CAPLUS

CN α -L-Mannopyranoside, 4-[1,3-bis(acetyloxy)-2-[4-[3-(acetyloxy)propyl]-2,6-dimethoxyphenoxy]propyl]-2-methoxyphenyl 6-deoxy-, triacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
Currently available stereo shown.



ACCESSION NUMBER: 2003:213284 CAPLUS
 DOCUMENT NUMBER: 138:382105
 TITLE: Phenolic compounds from *Nymphaea odorata*
 AUTHOR(S): Zhang, Zhizhen; ElSohly, Hala N.; Li, Xing-Cong; Khan, Shabana I.; Broedel, Sheldon E., Jr.; Raulli, Robert E.; Cihlar, Ronald L.; Burandt, Charles; Walker, Larry A.
 CORPORATE SOURCE: National Center for Natural Products, Research Research Institute of Pharmaceutical Sciences and Department of Pharmacology, School of Pharmacy, University of Mississippi, University, MS, 38677, USA
 SOURCE: Journal of Natural Products (2003), 66(4), 548-550
 CODEN: JNPRDF; ISSN: 0163-3864
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GRAPHIC IMAGE:



I

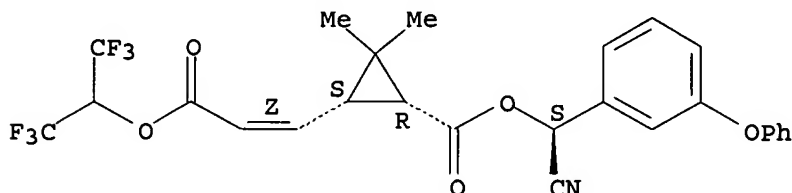
ABSTRACT:

Assay-guided fractionation of the ethanol extract of *Nymphaea odorata* resulted in the identification of two lignans, one new and one known, together with six known flavonol glycosides. The structures of the compds. were established by spectroscopic anal. as nymphaeoside A (I), icariside E4, kaempferol 3-O- α -L-rhamnopyranoside (afzelin), quercetin 3-O- α -L-rhamnopyranoside, myricetin 3-O- α -L-rhamnopyranoside (myricitrin), quercetin 3-O-(6''-O-acetyl)- β -D-galactopyranoside, myricetin 3-O- β -D-galactopyranoside, and myricetin 3-O-(6''-O-acetyl)- β -D-galactopyranoside. Three of the compds. showed marginal inhibitory effect against fatty acid synthase with IC₅₀ values of 45, 50, and 25 μ g/mL, resp.

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 5 OF 20 CAPLUS COPYRIGHT 2006 ACS on STN
 IT 101007-06-1, Acrinathrin
 RL: BUU (Biological use, unclassified); TEM (Technical or engineered material use); BIOL (Biological study); USES (Uses)
 (Ardent; cloth finishing agents containing active agents such as pesticides and antistatics and softeners, in absorptive materials used during drying by rotary dryer)
 RN 101007-06-1 CAPLUS
 CN Cyclopropanecarboxylic acid, 2,2-dimethyl-3-[(1Z)-3-oxo-3-[2,2,2-trifluoro-1-(trifluoromethyl)ethoxy]-1-propenyl]-, (S)-cyano(3-phenoxyphenyl)methyl ester, (1R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry as shown.



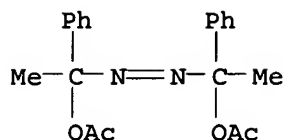
ACCESSION NUMBER: 2002:284623 CAPLUS
 DOCUMENT NUMBER: 136:296135
 TITLE: Cloth finishing agents used during drying by rotary dryer
 INVENTOR(S): Ichikawa, Masataka
 PATENT ASSIGNEE(S): Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 3 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2002114608	A2	20020416	JP 2000-307680	20001006
PRIORITY APPLN. INFO.:			JP 2000-307680	20001006

ABSTRACT:

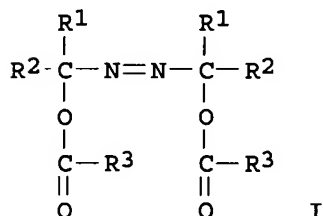
The agents are manufactured by impregnating absorptive materials with ≥ 1 selected from bactericides, fungicides, acaricides, antistatics, softeners, and ***perfumes.*** Soflan Color Foam (polyurethane foam sheet) was impregnated with a mixture of Irgasan DP 300 (triclosan), propylene glycol, and H₂O to give an antibacterial and antifungal finishing agent. Washed and dewatered bed sheets were dried in a rotary dryer together with the agents for 30 min. The drying process was repeated 90 times every day between May and Sept. No generation of bacteria and fungi was observed on the sheets and inside the dryer.

L7 ANSWER 6 OF 20 CAPLUS COPYRIGHT 2006 ACS on STN
 IT 57908-47-1
 RL: TEM (Technical or engineered material use); USES (Uses)
 (composition of foaming agent containing azoalkane derivs. for manufacturing foamed body)
 RN 57908-47-1 CAPLUS
 CN Benzenemethanol, α, α' -azobis[α -methyl-, diacetate (ester) (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1998:728421 CAPLUS
 DOCUMENT NUMBER: 130:40589
 TITLE: Composition of foaming agent containing azoalkane derivatives for manufacturing foamed body
 INVENTOR(S): Masatomi, Tsunehiko; Hikita, Shoji; Furuichi, Tomohiro
 PATENT ASSIGNEE(S): Otsuka Chemical Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 10298535	A2	19981110	JP 1997-123307	19970424
PRIORITY APPLN. INFO.:			JP 1997-123307	19970424
OTHER SOURCE(S):	MARPAT	130:40589		
GRAPHIC IMAGE:				



ABSTRACT:

The foaming agent comprises an azoalkane derivative having a general formula (I) where R¹ and R² can be the same or different and are lower alkyl or allyl groups and R³ is an alkyl or allyl group, an alkaline earth metal oxide, and a phosphate. The azoalkane can be 1,1'-azobis(1-acetoxy-1-phenylethane). Pungent odor such as acetic acid odor is prevented from attaching on foamed body manufactured by using the above foaming agent.

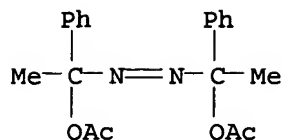
L7 ANSWER 7 OF 20 CAPLUS COPYRIGHT 2006 ACS on STN

IT 57908-47-1

RL: TEM (Technical or engineered material use); USES (Uses)
 (composition of foaming agent containing azoalkane derivs. for manufacturing foamed body)

RN 57908-47-1 CAPLUS

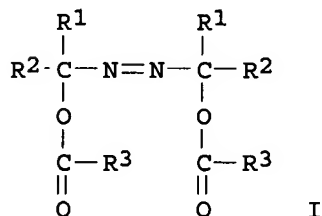
CN Benzenemethanol, α,α'-azobis[α-methyl-, diacetate
 (ester) (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1998:728420 CAPLUS
 DOCUMENT NUMBER: 130:40588
 TITLE: Composition of foaming agent containing azoalkane derivatives for manufacturing foamed body
 INVENTOR(S): Masatomi, Tsunehiko; Hikita, Shoji; Furuichi, Tomohiro
 PATENT ASSIGNEE(S): Otsuka Chemical Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 10298534	A2	19981110	JP 1997-123306	19970424
PRIORITY APPLN. INFO.:			JP 1997-123306	19970424
OTHER SOURCE(S):	MARPAT	130:40588		

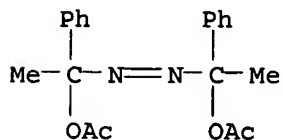
GRAPHIC IMAGE:



ABSTRACT:

The foaming agent comprises an azoalkane derivative having a general formula (I) where R¹ and R² can be the same or different and are lower alkyl or allyl groups and R³ is an alkyl or allyl group, and a compound which generates ammonia during heating. The azoalkane can be 1,1'-azobis(1-acetoxy-1-phenylethane). Pungent odor such as acetic acid odor is prevented from attaching on foamed body manufactured by using the above foaming agent.

L7 ANSWER 8 OF 20 CAPLUS COPYRIGHT 2006 ACS on STN
 IT 57908-47-1, 1,1'-Azobis(1-acetoxy-1-phenylethane)
 RL: MOA (Modifier or additive use); USES (Uses)
 (silicone rubber compns. containing azo blowing agent and H siloxane deodorants for sponges)
 RN 57908-47-1 CAPLUS
 CN Benzenemethanol, α,α'-azobis[α-methyl-, diacetate
 (ester) (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1997:368996 CAPLUS
 DOCUMENT NUMBER: 127:19317
 TITLE: Silicone rubber sponge compositions and their foamed and cured product sponges
 INVENTOR(S): Iida, Isao
 PATENT ASSIGNEE(S): Toshiba Silicone Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 09095552	A2	19970408	JP 1995-252163	19950929
JP 2869367	B2	19990310		

PRIORITY APPLN. INFO.: JP 1995-252163 19950929

ABSTRACT:

Title compns., which give sponges with good blowing, surface smoothness, small compression set, and no odor, contain $\text{RaSiO}(4\text{-a})/2$ ($\text{R} = \text{C1-10}$ hydrocarbyl; $\text{a} = 1.95\text{-}2.05$) 100, fillers 3-500, 1,1'-azobis(1-acetoxy-1-phenylethane) (I) 0.1-20, $\text{R1bHcXdSiO}(4\text{-b-c-d})/2$ ($\text{R1} = \text{hydrocarbyl}$; $\text{X} = \text{OH}$, hydrolyzable group; $\text{b}, \text{d} = 0\text{-}3$; $0 < \text{c} < 3$; $0 < \text{b} + \text{c} + \text{d} \leq 4$) 0.1-20, and organic peroxides 0.05-15 parts. Thus, 100 parts base compound comprising dimethylvinylsilyl-terminated di-Me, Me vinyl siloxane (di-Me siloxane 99.73 mol.%, Me vinyl siloxane 0.25 mol.%) 100, Aerosil 200 40, and OH-terminated di-Me siloxane 4 parts was mixed with I 5, Me₃Si-terminated Me H siloxane 1, 2,4-dichlorobenzoyl peroxide 0.2, and 2,5-bis(tert-butylperoxy)-2,5-dimethylhexane 0.5 part and extruded to give a sponge showing d. 0.32, good surface states, uniform microcells, compression set (180° + 22 h, 50% compression) 18, and no odor.

L7 ANSWER 9 OF 20 CAPLUS COPYRIGHT 2006 ACS on STN

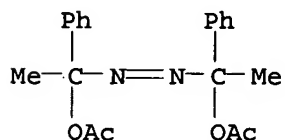
IT 57908-47-1, 1,1'-Azobis(1-acetoxy-1-phenylethane)

RL: MOA (Modifier or additive use); USES (Uses)

(silicone rubber compns. containing azo blowing agent and deodorants for sponges)

RN 57908-47-1 CAPLUS

CN Benzenemethanol, α,α' -azobis[α -methyl-, diacetate (ester) (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1997:368995 CAPLUS
 DOCUMENT NUMBER: 127:19316
 TITLE: Silicone rubber sponge compositions and their foamed and cured product sponges
 INVENTOR(S): Iida, Isao; Iijima, Hiroyoshi
 PATENT ASSIGNEE(S): Toshiba Silicone Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 09095551	A2	19970408	JP 1995-252162	19950929
JP 2869366	B2	19990310		
PRIORITY APPLN. INFO.:			JP 1995-252162	19950929

ABSTRACT:

Title compns., which give sponges with good blowing, surface smoothness, small compression set, and no odor, contain $\text{RaSiO}(4-a)/2$ ($R = \text{C1-10 hydrocarbyl}$; $a = 1.95-2.05$) 100, fillers 3-500, 1,1'-azobis(1-acetoxy-1-phenylethane) (I) 0.1-20, Group I or II metal oxides, hydroxides, or carbonates or hydrotalcites 0.01-10 parts, and curing agents. Thus, 100 parts base compound comprising dimethylvinylsilyl-terminated di-Me, Me vinyl siloxane (di-Me siloxane 99.73 mol.%, Me vinyl siloxane 0.25 mol.%) 100, Aerosil 200 40, and OH-terminated di-Me siloxane 4 parts was mixed with I 5, MgO 0.5, 2,4-dichlorobenzoyl peroxide 0.2, and 2,5-bis(tert-butylperoxy)-2,5-dimethylhexane 0.5 part and extruded to give a sponge showing d. 0.30, good surface states, uniform microcells, compression set ($180^\circ + 22 \text{ h}$, 50% compression) 17, and no odor.

L7 ANSWER 10 OF 20 CAPLUS COPYRIGHT 2006 ACS on STN

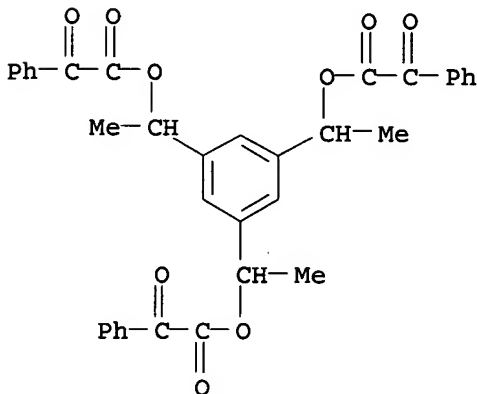
IT 183430-15-1P

RL: AGR (Agricultural use); BUU (Biological use, unclassified); PEP (Physical, engineering or chemical process); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)

(controlled release of mol. components comprising use of fragmenting and expanding mols.)

RN 183430-15-1 CAPLUS

CN Benzeneacetic acid, α -oxo-, 1,3,5-benzenetriyltriethylidene ester (9CI) (CA INDEX NAME)



ACCESSION NUMBER:

1996:701656 CAPLUS

DOCUMENT NUMBER:

125:339042

TITLE:

Controlled release of molecular components comprising the use of fragmenting and expanding molecules

INVENTOR(S):

Segalman, Daniel J.; Saunders, Randall S.; Wallace, J. Shield

PATENT ASSIGNEE(S):

Sandia Corporation, USA

SOURCE:

PCT Int. Appl., 51 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	-----

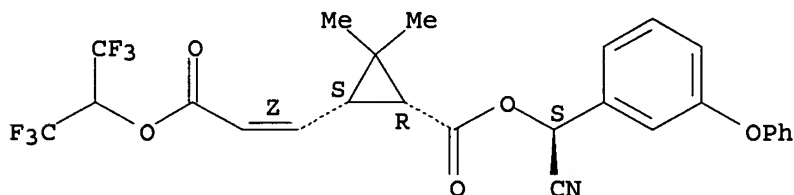
WO 9630002 A1 19961003 WO 1996-US4372 19960329
W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE,
ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT,
LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE,
SG, SI
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR,
IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML
US 5795581 A 19980818 US 1995-415352 19950331
AU 9657115 A1 19961016 AU 1996-57115 19960329
PRIORITY APPLN. INFO.: US 1995-415352 A 19950331
WO 1996-US4372 W 19960329

ABSTRACT:

A method for releasing mols. (guest mols.) from the matrix formed by the structure of another mol. (host mol.) in a controllable manner has been invested. Applications based on such mol. systems may revolutionize significant areas of medicine, in particular the treatment of cancer and of viral infection. Similar effects can also be obtained by controlled fragmentation of a source mol., where the mol. fragments form the active principle. An aromatic triketooester was subjected to UV radiation to break the polar CO bonds between the core mol. and the dendrimer branches, yielding triacetylbenzene, benzaldehyde, and CO as fragmentation products.

L7 ANSWER 11 OF 20 CAPLUS COPYRIGHT 2006 ACS on STN
IT 101007-06-1, Acrinathrin
RL: AGR (Agricultural use); BIOL (Biological study); USES (Uses)
(emulsified spray formulations)
RN 101007-06-1 CAPLUS
CN Cyclopropanecarboxylic acid, 2,2-dimethyl-3-[(1Z)-3-oxo-3-[2,2,2-trifluoro-1-(trifluoromethyl)ethoxy]-1-propenyl]-, (S)-cyano(3-phenoxyphenyl)methyl ester, (1R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



ACCESSION NUMBER: 1995:991038 CAPLUS
DOCUMENT NUMBER: 124:48346
TITLE: Emulsified spray formulations.
INVENTOR(S): Martin, Robert; Cayley, George R.; Thacker, Jonathan R. M.; Hall, Franklin R.; North, Denise K.; Groome, John M.; Jeffries, David A.
PATENT ASSIGNEE(S): Roussel-UCLAF, Fr.
SOURCE: U.S., 13 pp. Cont.-in-part of U.S. Ser. No. 979,452, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5466458	A	19951114	US 1994-196809	19940215
PRIORITY APPLN. INFO.:			US 1994-196809	B2 19940215
			US 1992-979452	B2 19921120
			US 1993-78212	B1 19930617

ABSTRACT:

A formulation suitable for spraying or for dilution with water to form a sprayable preparation, is given. The formulation comprises an active ingredient, optionally a carrier or solvent, an emulsifier and an evaporation retardant. The formulation satisfies the formula: (oil phase mass)/(retardant mass) \leq Moil/Mretardant + Exp[ln((L/4) + Cln(AXB))/C], where .

$L \leq 15$, $A = 700376$, $B = -1.51$, $C = 0.8472$, Moil is the weighted average relative molar mass of the oil phase Mretardant is the weighted average relative molar mass of the retardant, and $X = (\text{Moil})^{1.8}/Y$, where Y is the molar solubility ratio of the formulation, defined as the min. number of moles of the oil phase which will dissolve the retardant, divided by the number of moles of retardant, provided that, in the formula above, any solvent which has no liquid phase at 27° is excluded. The formulation may include a pesticide or herbicide. The action of the evaporation retardant is improved. Suitable evaporation retardants are 1-hexadecylamine, 1-heptadecylamine, 1-octadecylamine, or hexadecan-1-ol, optionally mixed with octadecan-1-ol. The formulation is usable for pesticides, dyes, drugs, paints, perfumes, textile finishes, etc.

L7 ANSWER 12 OF 20 CAPLUS COPYRIGHT 2006 ACS on STN

IT 170738-61-1P 170738-62-2P

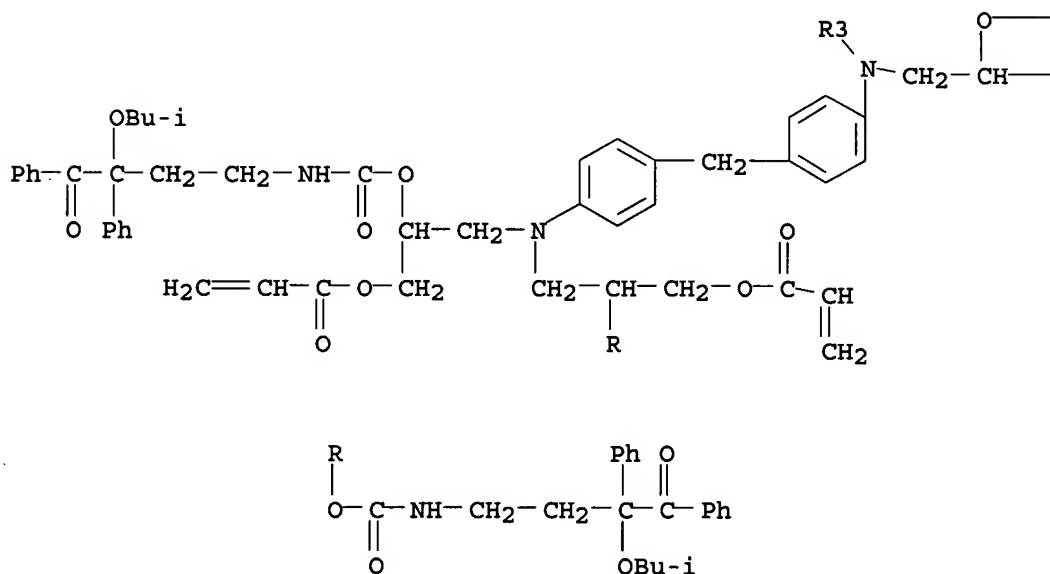
RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation); USES (Uses)

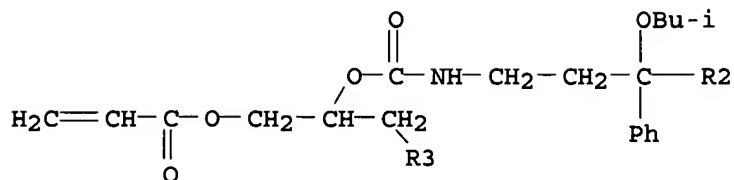
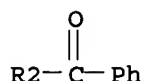
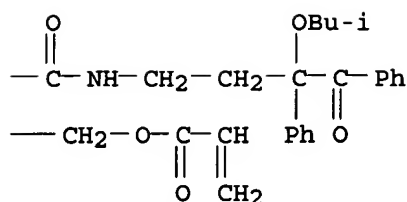
(photopolymn. initiators with good storability and compatibility and photocurable polymer compns. containing the same free from toxicity, odor, and decolorization)

RN 170738-61-1 CAPLUS

CN 2-Propenoic acid, methylenebis[4,1-phenylenenitrilobis[2-[[[3-(2-methylpropoxy)-4-oxo-3,4-diphenylbutyl]amino]carbonyl]oxy]-3,1-propanediyl]] ester (9CI) (CA INDEX NAME)

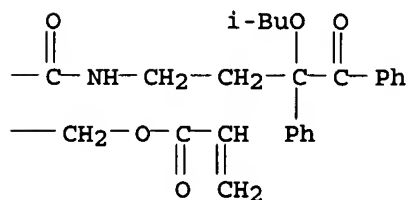
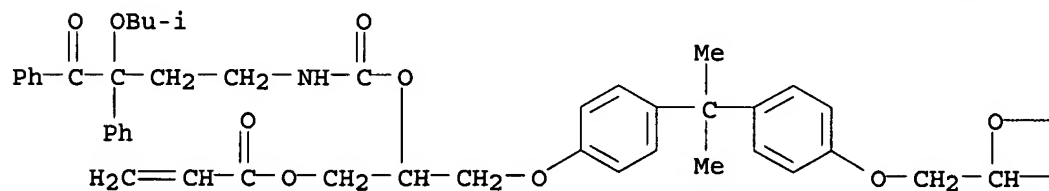
PAGE 1-A





RN 170738-62-2 CAPLUS

CN 2-Propenoic acid, (1-methylethylidene)bis[4,1-phenyleneoxy[2-[[[3-(2-methylpropoxy)-4-oxo-3,4-diphenylbutyl]amino]carbonyl]amino]-3,1-propanediyl]] ester (9CI) (CA INDEX NAME)



ACCESSION NUMBER:

1995:943501 CAPLUS

DOCUMENT NUMBER:

123 : 342164

TITLE:

Photopolymerization initiators with good storability and compatibility and photocurable polymer compositions containing the same free from toxicity, odor, and decolorization

PATENT ASSIGNEE(S) :

Korea Institute of Science and Technology, S. Korea

SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 07206775	A2	19950808	JP 1994-173835	19940726
KR 124966	B1	19971126	KR 1994-150	19940106
PRIORITY APPLN. INFO.:			KR 1994-150	A 19940106

ABSTRACT:

The title initiators are benzoin alkyl ethers chemical bonded to epoxy or epoxy acrylate prepolymers. A photoinitiator was prepared by reacting α -(2-isocyanatoethyl)benzoin iso-Bu ether with bisphenol A diglycidyl ether diacrylate and used for acrylates.

L7 ANSWER 13 OF 20 CAPLUS COPYRIGHT 2006 ACS on STN

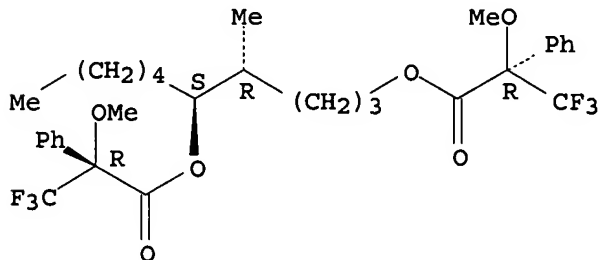
IT 165070-12-2P 165173-73-9P 165173-74-0P
 165173-75-1P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (preparation, resolution, and absolute configuration of methyldecanolide stereoisomers)

RN 165070-12-2 CAPLUS

CN Benzeneacetic acid, α -methoxy- α -(trifluoromethyl)-,
 2-methyl-1-pentyl-1,5-pentanediy l ester, [1S-[1R*(S*),2S*,5(S*)]]- (9CI)
 (CA INDEX NAME)

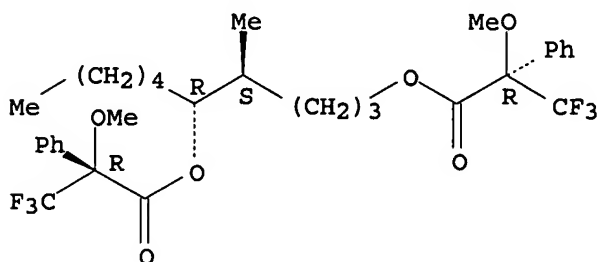
Absolute stereochemistry.



RN 165173-73-9 CAPLUS

CN Benzeneacetic acid, α -methoxy- α -(trifluoromethyl)-,
 2-methyl-1-pentyl-1,5-pentanediy l ester, [1R-[1R*(R*),2S*,5(R*)]]- (9CI)
 (CA INDEX NAME)

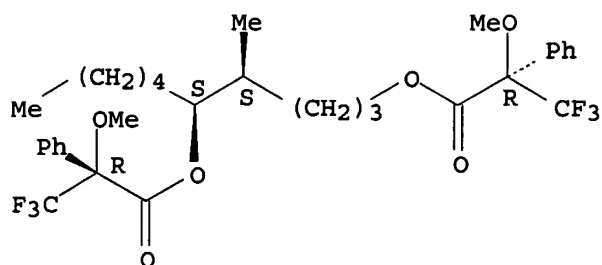
Absolute stereochemistry.



RN 165173-74-0 CAPLUS

CN Benzeneacetic acid, α -methoxy- α -(trifluoromethyl)-,
 2-methyl-1-pentyl-1,5-pentanediy l ester, [1S-[1R*(S*),2R*,5(S*)]]- (9CI)
 (CA INDEX NAME)

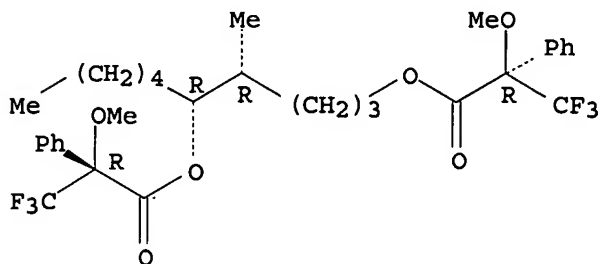
Absolute stereochemistry.



RN 165173-75-1 CAPLUS

CN Benzeneacetic acid, α -methoxy- α -(trifluoromethyl)-,
2-methyl-1-pentyl-1,5-pentanediy l ester, [1R-[1R*(R*),2R*,5(R*)]] - (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



ACCESSION NUMBER: 1995:577114 CAPLUS

DOCUMENT NUMBER: 123:83085

TITLE: Chiral compounds of essential oils XIX.

4-Methyl-5-decanolide: chirospecific analysis,
structure and properties of the stereoisomers

AUTHOR(S): Bartschat, Dietmar; Lehmann, Detmar; Dietrich, Armin;
Mosandl, Armin; Kaiser, Roman

CORPORATE SOURCE: Inst. Lebensmittelchemie, Biozentrum, Johann Wolfgang
Goethe-Univ. Frankfurt, Frankfurt/Main, 60439, Germany

SOURCE: Phytochemical Analysis (1995), 6(3), 130-4

CODEN: PHANEL; ISSN: 0958-0344

PUBLISHER: Wiley

DOCUMENT TYPE: Journal

LANGUAGE: English

ABSTRACT:

Racemic mixts. of synthetic cis- or trans-4-methyl-5-decanolide were separated by enantioselective high performance liquid chromatog. with Chiraspher-RT to yield all four stereoisomers as enantiopure compds. of distinct odor activities. In order to elucidate stereochem. features the isolated stereoisomers were reduced to their 4-methyl-1,5-decanediols with lithium aluminum hydride. Absolute configurations were derived from proton NMR studies of diastereomeric di-(R)-2-methoxy-2-trifluoromethylphenylacetic acid esters of these 1,5-diols. Using enantioselective multidimensional capillary gas chromatog., the direct enantioselective anal. of all four lactone stereoisomers was achieved. The application of this method to the scent of living, white flowering orchids (*Aerangis confusa*) proves cis-(4S)-methyl-(5S)-decanolide as the unique and genuine stereoisomer of *Aerangis* lactone.

L7 ANSWER 14 OF 20 CAPLUS COPYRIGHT 2006 ACS on STN

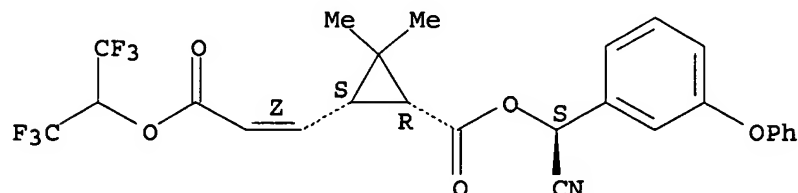
IT 101007-06-1

RL: BIOL (Biological study)

(solns. of, biphenyl derivative solvents for)

RN 101007-06-1 CAPLUS
 CN Cyclopropanecarboxylic acid, 2,2-dimethyl-3-[(1Z)-3-oxo-3-[2,2,2-trifluoro-1-(trifluoromethyl)ethoxy]-1-propenyl]-, (S)-cyano(3-phenoxyphenyl)methyl ester, (1R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry as shown.

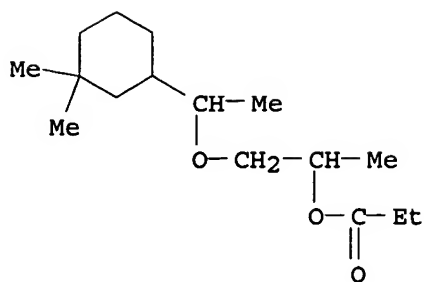


ACCESSION NUMBER: 1994:48134 CAPLUS
 DOCUMENT NUMBER: 120:48134
 TITLE: Pyrethroid solutions.
 INVENTOR(S): Audegond, Lilian; Lambert, Bernard
 PATENT ASSIGNEE(S): Roussel-UCLAF, Fr.
 SOURCE: Eur. Pat. Appl., 12 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: French
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

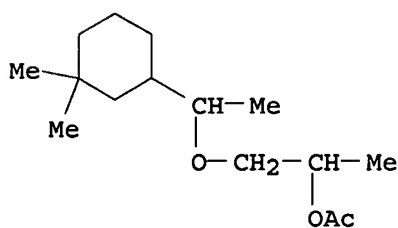
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 567368	A1	19931027	EP 1993-400923	19930408
EP 567368	B1	19970312		
R: CH, DE, FR, GB, IT, LI, NL				
FR 2689729	A1	19931015	FR 1992-4347	19920409
FR 2689729	B1	19940603		
US 5435992	A	19950725	US 1993-41843	19930402
BR 9301479	A	19931013	BR 1993-1479	19930407
AU 9336778	A1	19931014	AU 1993-36778	19930407
AU 665065	B2	19951214		
JP 06009320	A2	19940118	JP 1993-103675	19930407
PRIORITY APPLN. INFO.:			FR 1992-4347	A 19920409
OTHER SOURCE(S):	MARPAT 120:48134			

ABSTRACT:
 Solns. of pyrethroids in optionally-substituted biphenyls Ph₂(CHCHMe₂)_n (n = 0 or 1), such as BVA XK solvents, are nonirritant and have low odor.
 The solns. are especially suitable for household use.

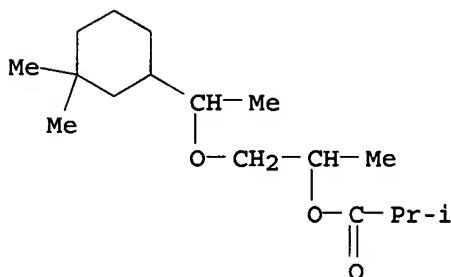
L7 ANSWER 15 OF 20 CAPLUS COPYRIGHT 2006 ACS on STN
 IT 141773-62-8P 141773-64-0P 141773-67-3P
 141773-72-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, as perfume fragrance)
 RN 141773-62-8 CAPLUS
 CN 2-Propanol, 1-[1-(3,3-dimethylcyclohexyl)ethoxy]-, propanoate (9CI) (CA INDEX NAME)



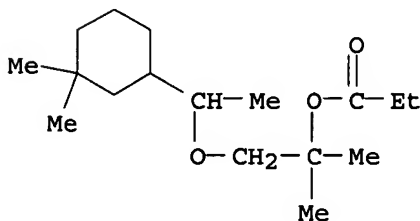
RN 141773-64-0 CAPLUS
 CN 2-Propanol, 1-[1-(3,3-dimethylcyclohexyl)ethoxy]-, acetate (9CI) (CA INDEX NAME)



RN 141773-67-3 CAPLUS
 CN Propanoic acid, 2-methyl-, 2-[1-(3,3-dimethylcyclohexyl)ethoxy]-1-methylethyl ester (9CI) (CA INDEX NAME)



RN 141773-72-0 CAPLUS
 CN 2-Propanol, 1-[1-(3,3-dimethylcyclohexyl)ethoxy]-2-methyl-, propanoate (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1992:407513 CAPLUS
 DOCUMENT NUMBER: 117:7513
 TITLE: Preparation of 4-cycloalkyl-3-oxapentyl alkanoates as perfume fragrances
 INVENTOR(S): Giersch, Wolfgang Klaus; Schulte-Elte, Karl Heinrich

PATENT ASSIGNEE(S): Firmenich S. A., Switz.
 SOURCE: Eur. Pat. Appl., 15 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: French
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 472966	A1	19920304	EP 1991-113240	19910807
EP 472966	B1	19940928		
R: CH, DE, FR, GB, LI, NL				
US 5166412	A	19921124	US 1991-741027	19910806
JP 06072952	A2	19940315	JP 1991-214881	19910827
JP 2974834	B2	19991110		

PRIORITY APPLN. INFO.: CH 1990-2799 A 19900828
 OTHER SOURCE(S): MARPAT 117:7513

ABSTRACT:

RCHMeOCR1R2CR3R4O2CR5 (R = 3,3-dimethylcyclopentyl, -cyclohexyl; when R1 = R2 = H, R3 and/or R4 = Me; when R3 = R4 = H, R1 and/or R2 = Me; R5 = alkyl) were prepared. Thus, 1-(3,3-dimethyl-1-cyclohexyl)-1-ethanone was ketalized by HOCH2CHMeOH and the dioxolane product reduced with Dibal to give RCHMeOCHMeCH2OR4 (I; R = 3,3-dimethylcyclohexyl) (II; R4 = H) and RCHMeOCH2CHMeOR4 (III; R same as I) (IV; R4 = H) as a mixture which was treated with EtCOCl to give II and IV (R4 = EtCO in each) as mixts. of diastereomers. ***Perfume*** formulations comprising title compds. are given.

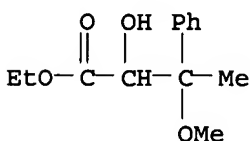
L7 ANSWER 16 OF 20 CAPLUS COPYRIGHT 2006 ACS on STN

IT 58671-12-8P 59717-84-9P 59717-85-0P
 59717-87-2P 59717-88-3P 59717-89-4P
 59717-90-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

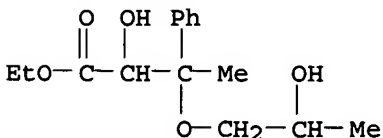
RN 58671-12-8 CAPLUS

CN Benzenepropanoic acid, α -hydroxy- β -methoxy- β -methyl-, ethyl ester (9CI) (CA INDEX NAME)



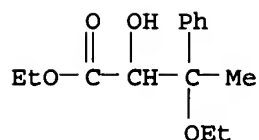
RN 59717-84-9 CAPLUS

CN Benzenepropanoic acid, α -hydroxy- β -(2-hydroxypropoxy)- β -methyl-, ethyl ester (9CI) (CA INDEX NAME)

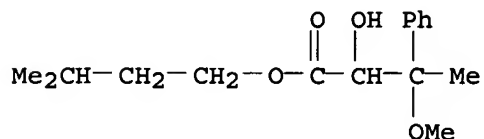


RN 59717-85-0 CAPLUS

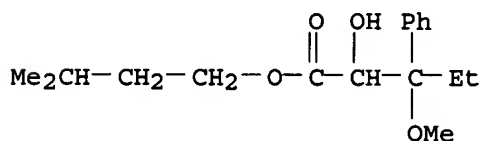
CN Benzenepropanoic acid, β -ethoxy- α -hydroxy- β -methyl-, ethyl ester (9CI) (CA INDEX NAME)



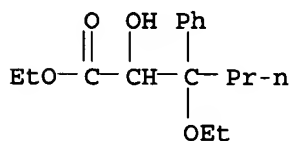
RN 59717-87-2 CAPLUS
 CN Benzenepropanoic acid, α -hydroxy- β -methoxy- β -methyl-,
 3-methylbutyl ester (9CI) (CA INDEX NAME)



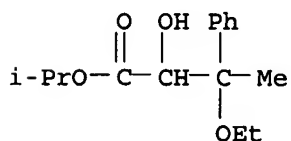
RN 59717-88-3 CAPLUS
 CN Benzenepropanoic acid, β -ethyl- α -hydroxy- β -methoxy-,
 3-methylbutyl ester (9CI) (CA INDEX NAME)



RN 59717-89-4 CAPLUS
 CN Benzenepropanoic acid, β -ethoxy- α -hydroxy- β -propyl-, ethyl
 ester (9CI) (CA INDEX NAME)



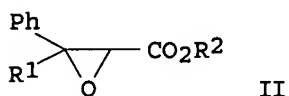
RN 59717-90-7 CAPLUS
 CN Benzenepropanoic acid, β -ethoxy- α -hydroxy- β -methyl-,
 1-methylethyl ester (9CI) (CA INDEX NAME)



ACCESSION NUMBER:	1976:432649 CAPLUS
DOCUMENT NUMBER:	85:32649
TITLE:	3-Phenylglyceric acid derivatives
INVENTOR(S):	Iijima, Hiroshi; Kawanobe, Tsuneo; Kogami, Kunio; Hayashi, Kazuo
PATENT ASSIGNEE(S):	Hasegawa, T., Co., Ltd., Japan
SOURCE:	Jpn. Kokai Tokkyo Koho, 8 pp. CODEN: JKXXAF
DOCUMENT TYPE:	Patent

LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

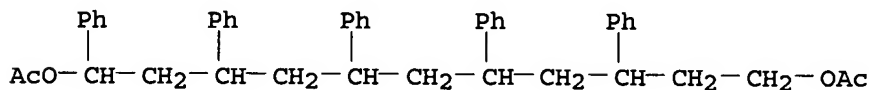
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 51004135	A2	19760114	JP 1974-71833	19740625
JP 57029445	B4	19820623		
PRIORITY APPLN. INFO.:			JP 1974-71833	A 19740625
GRAPHIC IMAGE:				



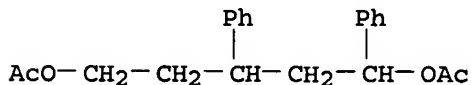
ABSTRACT:

Phenylglyceric acid derivs. $\text{PhCR}_1(\text{OR})\text{C}(\text{OH})\text{CO}_2\text{R}_2$ I (R = H, alkyl, polyhydric alc. group; R1 and R2 = H, alkyl) were prepared by epoxide cleavage of phenylglycidic acid derivs. II with H₂O and(or) alcs. at \geq apprx.30°. Lower temps. greatly decreased the yield and reaction even at >50° caused no rearrangement to α -keto esters. I had a strawberry-like flavor. Thus, II (R1 = Me, R2 = Et) was stirred with 98% H₂SO₄ in H₂O at 60-70° for 0.5 hr to give 71.5% I (R = H, R1 = Me, R2 = Et) a mixture of the threo and erythro isomers, vs. 25% for reaction at 15°. Propylene glycol-EtOH-H₂O (1:1:1) as the solvent gave mixed I (R1 = Me, R2 = Et) where R = CH₂CHMeOH, (an erythro-threo mixture). Among 11 more I prepared were (R, R1, and R2 given): Bu, H, Bu; Me, Me, isoamyl; Me, Et, isoamyl; Et, Pr, Et.

L7 ANSWER 17 OF 20 CAPLUS COPYRIGHT 2006 ACS on STN
IT 859324-70-2, 1,11-Undecanediol, 1,3,5,7,9-pentaphenyl-, diacetate
872807-61-9, 1,5-Pentanediol, 1,3-diphenyl-, diacetate
(preparation of)
RN 859324-70-2 CAPLUS
CN 1,11-Undecanediol, 1,3,5,7,9-pentaphenyl-, diacetate (5CI) (CA INDEX NAME)



RN 872807-61-9 CAPLUS
CN 1,5-Pentanediol, 1,3-diphenyl-, diacetate (5CI) (CA INDEX NAME)



ACCESSION NUMBER: 1952:17703 CAPLUS
DOCUMENT NUMBER: 46:17703
ORIGINAL REFERENCE NO.: 46:3074f-i,3075a
TITLE: Cyclohexyl-substituted α,ω -glycols
INVENTOR(S): Arnold, Harold W.
PATENT ASSIGNEE(S): E. I. du Pont de Nemours & Co.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1

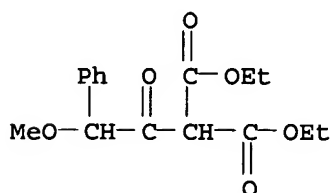
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2555912		19510605	US 1948-44992	19480818

ABSTRACT:

Cyclohexyl-substituted α,ω -glycols (I) are obtained by hydrogenation of the corresponding Ph-substituted α,ω -glycols with a Ru catalyst preferably at 80-120°. Thus, HOCH₂CH₂CHPhOH (II), nD₂₅ 1.5440, 100, 95% EtOH 39, and RuO₂ 2 are treated 2 hrs. with agitation at 100° with H at 1000-2000 lb./sq. in. pressure, and the cooled mixture filtered and fractionated to give HOCH₂CH₂CH(OH)C₆H₁₁ (III) 87 parts, colorless, slightly viscous oil, b_{2.5} 137-40°, nD₂₅ 1.4850. III and PhNCO give the bis-(phenylurethan), crystals; m. 115-16° (from C₆H₆-petr. ether). III heated 24 hrs. at 260° in a sealed tube does not change color and viscosity. To paraformaldehyde 60 and BF₃ 68 in AcOH 734.3 is added, with ice-cooling over a period of 1 min., PhCH:CH₂ 520, the mixture let stand 3 days at room temperature, then ice and NaOH 160 in H₂O 160 added, the resulting oily product separated, washed with H₂O, dried with CaSO₄, and distilled to give AcOCH₂(CH₂CHPh)₂OAc (IV) 21.4, b_{0.6} 183-8°, nD₂₅ 1.5341, and a still residue of crude AcOCH₂(CH₂CHPh)₂OAc 285.4 parts. IV 18.3 is refluxed with NaOH 40 in H₂O 40 and EtOH, the mixture extracted with PhMe, and the extract distilled to give HOCH₂(CH₂CHPh)₂OH (V) 12 parts, highly viscous liquid, b_{0.5} 200°. Hydrogenation of V 5.8 as above yields 1,3-dicyclohexyl-1,5-pentanediol 4.0 parts, highly viscous, colorless liquid, b₁ 178-92°, nD₂₅ 1.4988. C₆H₁₁CH(OH)CH₂OH (87%) is obtained similarly by hydrogenation of PhCH(OH)CH₂OH. Similar hydrogenation of II 150 with a Ni-on-kieselguhr catalyst at 180-90° yields Ph(CH₂)₃OH 73.6 parts, b_{2.4} 88°, nD₂₅ 1.5216 (p-nitrobenzoate, m. 48°). The I are useful intermediates for polyesters plasticizers, hydraulic fluid components, insect repellents, ***perfume*** ingredients, dust-collecting aids, and in the synthesis of organic compds.

L7 ANSWER 18 OF 20 CAPLUS COPYRIGHT 2006 ACS on STN
 IT 855658-51-4, Malonic acid, (methoxyphenylacetyl)-, diethyl ester
 (Mannich reaction with, and products therefrom)
 RN 855658-51-4 CAPLUS
 CN Malonic acid, (methoxyphenylacetyl)-, diethyl ester (5CI) (CA INDEX NAME)



ACCESSION NUMBER: 1952:8544 CAPLUS
 DOCUMENT NUMBER: 46:8544
 ORIGINAL REFERENCE NO.: 46:1513d-i,1514a-i,1515a-c
 TITLE: Alkyl- β -cyano- α -hydroxycinnamates and pyrrolidinetrienes
 AUTHOR(S): Skinner, Glenn S.; Gladner, Jules A.; Heitmiller, Richard F.
 CORPORATE SOURCE: Univ. of Delaware, Newark
 SOURCE: Journal of the American Chemical Society (1951), 73, 2230-3
 CODEN: JACSAT; ISSN: 0002-7863
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable

GRAPHIC IMAGE:

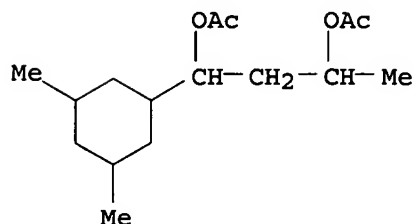
For diagram(s), see printed CA Issue.

ABSTRACT:

PhCHMe₂ (230 g.), 46.5 g. paraformaldehyde (I), and 46.4 g. ZnCl₂ were treated 4 hrs. at 50-5° in the usual way under a rapid stream of HCl, the mixture washed several times with ice-cold H₂O (with addition of petr. ether, to aid separation of the layers), the ether solution neutralized with NaOH, washed, anhydrous Na₂SO₄ added in small parts to break up the emulsion, and the organic layer shaken with excess anhydrous CaCl₂ to which 0.5 ml. saturated NaOH was added; distillation of the dried product gave (1) 84 g. (chloromethyl)isopropylbenzenes, b₁₉ 116-20°, (2) 9 g., b. 150-70°, and (3) 38.0 g. residue. PhEt (6 moles), 2.43 moles I, and 0.53 mole ZnCl₂ in 2 hrs. at 55° gave (1) 155 g. (chloromethyl)ethylbenzenes, b₁₆ 104-8°; (2) 32 g., b₁₆ 180-5°, and (3) 50 g. residue. With 3 moles PhEt, I 30 min. at 60°, yielded (1) 115 g., (2) 58 g., and (3) 50 g. PhCMe₃ (3.25 moles), 1.33 moles I, and 0.29 mole ZnCl₂ 90 min. at 50° gave (1) 179 g. (chloromethyl)-tert-butylbenzenes, b_{16.5} 119-21°, (2) 16 g., b₁₆ 150-60°, and (3) 5.5 g. residue. The (chloromethyl) compds. (1.2 moles) added over 45 min. to 188 ml. alcohol, 1.53 moles NaCN, and 68 ml. H₂O, and the mixture refluxed 5 hrs., gave the corresponding (alkylphenyl)acetonitrile mixts., p- and o-RC₆H₄CH₂CN: R = Et, b₁₉ 140-3° (88%); Me₂CH, b_{14.5} 134-7° (84.4%); Me₃C, b₁₅ 143-6° (90.5%). The alkyl-β-cyano-α-hydroxycinnamates (customarily called (alkylphenyl)cyanopyruvates) were made in the same general fashion as previously described (C.A. 43, 1746f), but separation of the isomers was more involved. The ether solution of the mixture of isomeric EtC₆H₄C(CN):C(OH)CO₂Et from 1.06 moles nitriles gave, after removal of the last solvent, finally with a capillary under reduced pressure, at 95-100°, 231 g. residue, which was treated in 100 ml. PhMe with 125 ml. petr. ether, let stand several hrs. in an ice bath, and the precipitate filtered, washed with 1:1 PhMe-petr. ether, and then petr. ether to give 115 g. product, m. 77-83°. This in 57 ml. PhMe cooled in a salt-ice bath gave a precipitate which, washed with ice-cold 1:1 PhMe-petr. ether, gave 101 g. p-isomer, m. 82-3°. Removal of the solvent from the 1st filtrate gave a viscous residue which largely solidified after 2 weeks, and removal of the liquid by suction for 2 days gave 76.5 g. crystals which, dissolved in 15 ml. hot EtOH and refrigerated, yielded 53.0 g., m. 50-60°; recrystn. from PhMe-petr. ether several times gave 23.4 g. o-isomer, m. 66-7°. Similarly 102 g. material m. 53-8° was isolated by freezing in Dry Ice-Me₂CO a solution in 25 ml. PhMe + 25 ml. petr. ether of the viscous residue from the p-isomer; solution in 25 ml. hot EtOH, cooling in a salt-ice bath, and filtering cold with the aid of a rubber dam gave 37.5 g., m. 59-62°, which, dissolved in 18 ml. hot PhMe, cooled in ice, filtered cold with suction, and washed with PhMe-petr. ether and petr. ether, gave 21 g., m. 66-7°. The esters (201 g.) obtained from 150 g. Me₂CHC₆H₄CH₂CN isomers by addition of 50 ml. ether plus 125 ml. petr. ether to the acidified reaction mixture, m. 60-71°. The viscous oil (31.8 g.) from the filtrate solidified and gave the p-isomer, m. 78-9°. The crude product in 200 ml. PhMe, treated with an equal volume of petr. ether added after it cooled a little, precipitated the p-isomer. The solvents were removed and the process repeated several times. After 112 g. p-isomer had collected, a finely divided precipitate appeared at room temperature and gave 3.0 g., m. 115.5-16.5°; the process was repeated and the combined crops of o-isomer recrystd. from PhMe. After all the o-compound was removed, more p-isomer (20.9 g.) was obtained. Total yield: 132.9 g. p- and 11.9 g. o-compound. The esters from 284.6 g. Me₃CC₆H₄CH₂CN isomers were obtained as an oil which was dissolved in 120 ml. hot PhMe and into the partially cooled solution was stirred 287 ml. petr. ether to precipitate 188.7 g., m. 70.5°, after washing with PhMe-petr. ether and petr. ether; removal of the solvents and repetition of the process with 70 ml. PhMe and 140 ml. petr. ether gave an addnl. 130 g., m. 72-4°. Reworking the filtrate 4 times gave a total of 369.7 g. which, recrystd. from 1:2 PhMe-petr. ether, gave pure p-isomer, m. 74-5°. The o-isomer could not be isolated from

the 72.4 g. oil residue. The pure esters (0.15 mole) when stirred and heated with 0.16 mole NaOH in 200 ml. H₂O dissolved at 50-70°; heating was discontinued when a precipitate formed at 70-80°. After the nitriles were separated with ether, the H₂O layer was heated with 1.6 g. NaOH, giving the RC₆H₄CH₂CN as colorless liquids with pleasant odors, hydrolyzed to the RC₆H₄CH₂CO₂H by refluxing 0.1 mole 5 hrs. with 13 g. 40% aqueous NaOH in 75 ml. EtOH. The % yields of unbrominated 4-(alkylphenyl)-2,3,5-pyrrolidinetriones obtained by cyclization of the RC₆H₄C(CN):C(OH)CO₂Et as previously described (C.A. 43, 1746f) were: R = p-Et 80, p-Me₂CH 81, p-Me₃C, 58 (recrystd. from hot EtOH). o-EtC₆H₄C(CN):C(OH)CO₂Et (0.02 mole), heated 6 hrs. at 50° with 0.02 mole Br and 0.02 mole H₂O in 16 ml. CHCl₃, let stand 2 days at room temperature, and concentrated gave 3.7 g. unbrominated product, m. 149-53° (155-6° from CHCl₃). When the same amts. of reagents were dissolved in a min. amount of CHCl₃, a solid soon precipitated out; after 2 days at room temperature it required 50 ml. hot CHCl₃ for solution and fractional crystallization gave 2.8 g. very difficultly soluble 4-(4-bromo-2-ethylphenyl)pyrrolidinetrione and 1.3 g. very soluble 4-(o-ethylphenyl)pyrrolidinetrione. o-Me₂CHC₆H₄C(CN):C(OH)CO₂Et (0.02 mole) in 16 ml. CHCl₃ similarly treated gave a solid precipitate; the viscous residue after removal of the CHCl₃ in vacuo crystallized from CHCl₃ to give 4.5 g. crude lemon-yellow 4-(o-isopropylphenyl)pyrrolidinetrione, m. 186-7° (after several crystns.). On repetition with the minimum amount (6 ml.) of solvent, 1.0 g. crystals separated after 1 day; they contained Br and repeated crystallization from CHCl₃ gave 0.1 g., m. 194-6°, probably the brominated pyrrolidinetrione. 4-(p-ethylphenyl)pyrrolidinetrione (6.51 g.) heated to boiling in 1.84 g. KOH and 20 ml. H₂O and allowed to cool gave 4.9 g. p-EtC₆H₄CH₂CONH₂, m. 199-200° (from boiling EtOH), identified by alkaline hydrolysis to the acid, m. 89-90° (from hot EtOH). 4,2-BrEtC₆H₃CH₂CONH₂ (0.5 g.) refluxed 3 hrs. with 0.16 g. NaOH in 10 ml. EtOH gave the acid, m. 87-8° (from ligroine), oxidized to 4,1,2-BrC₆H₃(CO₂H)₂, m. 176-8°, by alkaline permanganate. o-Me₂CHC₆H₄CH₂CONH₂ (0.5 g.) was incompletely (50-60%) hydrolyzed after 5 hrs. under the above conditions to the acid, m. 58-9° (from ligroine) (neutralization equivalent 178 calculated, 170 found); oxidation with permanganate gave phthalic acid, m. 208-10°. The infrared spectrograms of the o- and p-MeC₆H₄C(CN):C(OH)CO₂Et both show absorption for the ethylenic double bond (6.2 μ) and 1 carbonyl group (5.8 μ) in harmony with PhC(CN):C(OEt)CO₂Et. The ether gives a very definite absorption for the nitrile group (4.6 μ) which is almost entirely absent in the cyanohydroxycinnamates. In the latter there is also an indication of a bonded OH at 3.0 μ. This suggests that the enols may have the structure (II). Et alkyl-β-cyano-α-hydroxycinnamates, RC₆H₄C(CN):C(OH)CO₂Et (R, m.p.): o-Me 115-17°; o-Et, 66-7°; o-Me₂CH, 115.5-16.5°; p-Me, 88-9°; p-Et, 82-3°; p-Me₂CH, 78-9°; p-Me₃C, 74-5°. Nitriles, RC₆H₄CH₂CN [R, b.p. (°C./5 mm.), yield (%), d₄²⁵]: o-Et, 95-7° (2 mm.), 69, -; p-Et, 100-1°, 95, 0.9775; p-Me₂CH, 106-8°, 77, 0.9631; p-Me₃C, 119-21°, 79, 0.9581. Pyrrolidinetriones, RCH.CO.NH.CO.CO (R, m.p., °C): o-MeC₆H₄, 186-7°; o-EtC₆H₄, 155-6°; o-Me₂CHC₆H₄, 186-7°; p-BrC₆H₄, 239-40°; 4,2-BrMeC₆H₃, 237.5-8.5°; 4,2-BrEtC₆H₃, 179-80°; p-MeC₆H₄, 263-4°; p-EtC₆H₄, 246-7°; p-Me₂CHC₆H₄, 232-3°; p-Me₃CC₆H₄, 249-50°. Amides, RCH₂CONH₂ [R, m.p. (°C), m.p. (°C) of acid]: o-EtC₆H₄, 128-9°, 83-4°; o-Me₂CHC₆H₄, 121-2°, 58-9°; 4,2-BrEtC₆H₃, 143-4°, 87-8°; p-EtC₆H₄, 199-200°, 89-90°; p-Me₂CHC₆H₄, 172-3°, 51-2°; p-Me₃CC₆H₄, 129-30°, 78-9°.

RN 860704-55-8 CAPLUS
 CN 1,3-Butanediol, 1-(3,5-dimethylcyclohexyl)-, diacetate (5CI) (CA INDEX NAME)



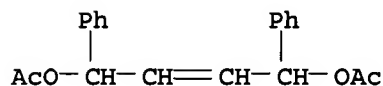
ACCESSION NUMBER: 1949:4599 CAPLUS
 DOCUMENT NUMBER: 43:4599
 ORIGINAL REFERENCE NO.: 43:1058c-h
 TITLE: Dialkylcyclohexyl glycols and derivatives
 INVENTOR(S): Sokal, Edward C.; Morris, Rupert C.
 PATENT ASSIGNEE(S): Shell Development Co.
 DOCUMENT TYPE: Patent
 LANGUAGE: Unavailable
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	-----
US 2449956		19480921	US 1945-604104	19450709

ABSTRACT:

3,5-Dialkylcyclohexyl glycols, in which the dialkylcyclohexyl group is directly attached to a C atom bearing one of the OH groups and in which the 2 OH groups are in the 1,3-positions relative to each other on C atoms in a side chain of at least 4 C atoms, their carboxylic acid esters, and their ethers are obtained by treating a conjugated diene with an α,β -unsatd. carbonylic compound, condensing the unsatd. cyclic carbonylic compound thus formed with a ketone, and treating the product with H in the presence of a hydrogenation catalyst. Examples of the resulting new compds. are: (1) 1-(3,5-Dimethylcyclohexyl)-1,3-butanediol, heavy viscous liquid, b1.5 127-8°, very slowly crystallizing to a white solid, m. 93-6°, miscible with hydrocarbon solvents such as kerosene, insol. in water, d204 of the liquid 1.00, n20D 1.4478, obtained from 2-methyl-1,3-pentadiene, acrolein, and acetone. (2) 1-(1,3,5-Trimethylcyclohexyl)-1,3-butanediol, from methylpentadiene, methacrolein, and acetone, colorless liquid, b0.5 103-6°. (3) (1,5-Dimethylcyclohexyl) (2,4,4-trimethyl-6-hydroxycyclohexyl)carbinol from pentadiene, methacrolein, and 3,3,5-trimethylcyclohexanone. (4) 1-(1-Methyl-2,5-endomethylenecyclohexyl)-1,3-butanediol, from cyclopentadiene, methacrolein, and acetone. (5) 1-(1-Methyl-6-ethyl-2,5-endomethylenecyclohexyl)-1,3-pentanediol from cyclopentadiene, EtCH:CMcCHO, and MeCOEt. (6) Diacetate of (1), from (1) with AcOH. (7) Di-Me ether, from (1) with Na metal and Me2SO4. (8) 1-Cyclohexyl-1,3-butanediol, prepared from butadiene, acrolein, and acetone, with subsequent hydrogenation of the 1-cyclohexenylbutan-1-ol-3-one first formed, a viscous water-white liquid, b0.5 100-3°. The products are useful as insect repellents, as constituents of printing inks for preventing too rapid drying of the ink, for making textile fibers more flexible, increasing their stretching properties, and softening them. Glyptal resins can also be obtained from these glycols, particularly oil-soluble ones, by their reaction with dibasic acids. Many other applications, e.g. as solvents for nitrocellulose, etc., as antifoaming agents, as intermediates for the production of plasticizers, ***perfume*** esters, and the like are also possible.

(preparation of)
 RN 94580-72-0 CAPLUS
 CN 2-Butene-1,4-diol, 1,4-diphenyl-, diacetate (7CI) (CA INDEX NAME)



ACCESSION NUMBER: 1924:10895 CAPLUS
 DOCUMENT NUMBER: 18:10895
 ORIGINAL REFERENCE NO.: 18:1467g-i
 TITLE: Octyl mercaptan
 AUTHOR(S): Kahn, Herman
 SOURCE: But. soc. chim. Roumania (1923), 5, 70-2
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable

ABSTRACT:
 Ploiesti benzine (d. 0.7860) on fractionation and purification with 10% H2SO4 and concentrated H2SO4 and HNO3 to remove aromatic compds., washing with H2O and distillation over Na gave a colorless liquid corresponding to C8H18, d15 0.7264, b. 121-3°. On treatment of this in vapor form with gaseous Cl, a colorless liquid was obtained, d15, 0.8526, b. 172-5°, which in turn on treatment with saturated alc. KSH, washing with H2O and distillation over CaCl2, gave octyl mercaptan, b. 198-200°, disagreeable odor, soluble in KOH, EtOH and Et2O, insol. in H2O, decomposed on warming to octyl sulfide and H2S and forms with alc. HgCl2 a white precipitate very difficult to dissolve in acids.

=> log y

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION

FULL ESTIMATED COST

██████████ ██████████

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION

CA SUBSCRIBER PRICE

██████████ ██████████

STN INTERNATIONAL LOGOFF AT 19:48:39 ON 19 MAR 2006